Listing of Claims:

1. (Previously Presented) A molecular reaction characteristic predicting method for predicting a reaction characteristic of a molecule, said method comprising the steps of:

setting a molecule surrounding surface surrounding the molecule so as to be reflected in a spatial dimension of the molecule, and assuming that a space surrounded by said molecule surrounding surface is a molecule surrounding space;

dividing said molecule surrounding space into a plurality of component spaces, by which a reaction characteristic of said molecule is characterized, in accordance with a predetermined space dividing procedure, and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces, said molecule surrounding space being divided so [as] that each component space of the plurality of component spaces includes therein each one atom composing the molecule;

assuming that a portion of each of said component surrounding surfaces appearing outside on said molecule surrounding surface is a frontier surrounding surface of each of said component spaces;

providing probe points on said frontier surrounding surface of each of said component spaces at regular intervals,

deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule. for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component spaces, as an electrostatic factor of said corresponding one of said component spaces;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces,

and deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said component sauces, as a steric factor of said corresponding one of said component spaces;

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces,

deriving the reaction characteristic values for all the component spaces of a predicting molecule of which a reaction characteristic is to be predicted,

forming a predicting vector having a plurality of vector components selected from the reaction characteristic values of the predicting molecule,

selecting a plurality of data molecules, a reaction characteristic of each of the data molecules being known,

deriving, the reaction characteristic values for all the component spaces of each of the data molecules,

forming a data vector for each of the data molecules, the data vector being corresponding to the predicting vector and having a plurality of vector components selected from the reaction characteristic values of each of the data molecules,

estimating a Euclid distance between the predicting vector and each data vector and getting a plurality of Euclid distances between the predicting vector and all the data molecules, and

predicting the reaction characteristic of the predicting molecule to be that the reaction characteristic of the predicting molecule is more similar to a reaction characteristic of a data molecule related to a shorter Euclid distance.

2. (Original) A molecular reaction characteristic predicting method as set forth in claim 1, wherein said molecule surrounding surface is an outermost contour enveloping surface formed by a plurality of atomic spherical surfaces, each of which extends around the center of each of said atoms of said molecule.

3. (Cancelled)

4. (Currently Amended) A molecular reaction characteristic predicting method [as set forth in claim 3,] <u>for predicting a reaction characteristic of a molecule. said method comprising the steps of:</u>

setting a molecule surrounding surface surrounding the molecule so as to be reflected in a spatial dimension the molecule, and assuming that a space surrounded by said molecule surrounding surface is a molecule surrounding space;

dividing said molecule surrounding space into a plurality of component spaces. by which reaction characteristic of said molecule is characterized in accordance with a predetermined space dividing procedure and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces said molecule surrounding space being divided so as that each component space of the plurality of component spaces includes therein each one atom composing the molecule;

assuming that a portion of each of said component surrounding surfaces appearing outside on slid molecule surrounding surface is a frontier surrounding surface of each of said component spaces;

wherein each of atomic spherical surfaces is derived so as to extend around the center of each of said atoms of said molecule, and wherein it is assumed that a portion of each of said atomic spherical surfaces intersecting other atomic spherical surfaces is an interior spherical surface and that a portion of each of said atomic spherical surfaces other than said interior spherical surface is a frontier spherical surface,

each of said component spaces being a space surrounded by a surface, which cuts said interior spherical surface, and said frontier spherical surface,

providing-probe points on said frontier surrounding surface of each of said component spaces at regular intervals:

deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component spaces, as an electrostatic factor of said corresponding one of said component spaces;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has predetermined steric characteristic. and all of said atoms of said molecule. for

each of said probe points on said frontier surrounding surface of each of said component spaces. and deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said component spaces, as a steric factor of said corresponding one of said component spaces;

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces,

deriving the reaction characteristic values for all the component spaces of a predicting molecule of which a reaction characteristic is to be predicted,

forming a predicting vector having a plurality of vector components selected from the reaction characteristic values of the predicting molecule,

selecting a plurality of data molecules, a reaction characteristic of each of the data molecules being known.

deriving the reaction characteristic values for all the component spaces of each of the data molecules,

forming a data vector for each of the data molecules, the data vector being corresponding to the predicting vector and having a plurality of vector components selected from the reaction characteristic values of each of the data molecules,

estimating a Euclid distance between the predicting vector and each data vector and getting a plurality of Euclid distances between the predicting vector and all the data molecules, and

predicting the reaction characteristic of the predicting molecule to be that the reaction characteristic of the predicting molecule is more similar to a reaction characteristic of a data molecule related to a shorter Euclid distance.

5. (Currently Amended) A molecular reaction characteristic predicting method as set forth in claim [1] 4, wherein [each of atomic spherical surfaces is derived so as to extend around the center of each of said atoms of said molecule, and wherein it is assumed that a portion of each of said atomic spherical surfaces intersecting other atomic spherical surfaces is an interior spherical surface and that a portion of each of said atomic spherical surfaces other than said interior spherical surface is a frontier spherical surface] said frontier surrounding surface is said frontier spherical surface.

6. (Original) A molecular reaction characteristic predicting method as set forth in claim 1, wherein each of atomic spherical surfaces is derived so as to extend around the center of each of said

atoms of said molecule, and wherein each of said atomic spherical surfaces is a spherical surface having a van der Waals radius of each of said atoms or a radius which is obtained by commonly adding a predetermined thickness to said van der Waals radius of each of said atoms.

7. (Original) A molecular reaction characteristic predicting method as set forth claim 1, wherein said molecule surrounding surface is a surrounding surface which surrounds a space formed by the frontier molecular orbital of said molecule.

8. (Original) A molecular reaction characteristic predicting method as set forth in claim l, wherein said predetermined space dividing procedure comprises the Voronoi division of said molecule surrounding space using the center of each of said atoms of said molecule as a mother point, and each of said component spaces is a Voronoi region formed by said Voronoi division.

9. (Original) A molecular reaction characteristic predicting method as set forth in claim l, wherein said space occupied rate is based on a volume of each of said component spaces.

10. (Original) A molecular reaction characteristic predicting method as set forth in claim 1, wherein said space occupied rate is based on the number of said probe points existing on said frontier surrounding surface.

11. (Original) A molecular reaction characteristic predicting method as set forth in claim 1, wherein said space occupied rate is based on an area of said frontier surrounding surface.

12. (Original) A molecular reaction characteristic predicting method as set forth in claim 1, wherein said electrostatic factor is normalized by dividing said sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component spaces by said space occupied rate of said corresponding one of said component spaces, and said steric factor is normalized by dividing said sum of said van der Waals energies on said frontier surrounding surface of a corresponding one of said component spaces by said space occupied rate of said corresponding one of said component spaces.

13. (Original) A molecular reaction characteristic predicting method as set forth in claim 1, wherein said probe atom is an sp^3 carbon, an sp^2 carbon or an sp carbon.

14. (Previously Presented) A molecular reaction characteristic predicting method as set forth in claim 1, which further comprises the steps of:

processing the plurality of data vectors for the data molecules in accordance, with a technique of a self-organizing neural network to display the processed result on a reaction characteristic

predicting map indicative of reaction characteristics of said plurality of molecules, and

predicting the reaction characteristic of the predicting molecule based on the map.

15. (Cancelled)

16. (Original) A molecular reaction characteristic predicting method as set forth in claim 14, wherein said self-organizing neural network is a Kohonen neural network, and said reaction characteristic predicting map is a Kohonen map.

17. (Original) A molecular reaction characteristic predicting method as set forth in claim 16, wherein said Kohonen map is displayed so as to be plane.

18. (Previously Presented) A molecular reaction characteristic predicting method comprising the steps of:

describing atomic spherical surfaces, each of which surrounds a corresponding one of atoms of the molecule;

assuming that a portion of each of said atomic spherical surfaces intersecting the atomic spherical surfaces of other atoms of said molecule is an interior spherical surface;

assuming that a portion of each of said atomic spherical surfaces other than said interior spherical surface is a frontier spherical surface, the frontier spherical surface being appeared outside;

providing probe points on each of said atomic spherical surfaces at regular intervals;

deriving a rate of occupied space as a space occupied rate of a corresponding one of said atoms, for each of said atoms;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of said atoms of said molecule, for each of said probe points on said frontier spherical surface of each of said atoms;

deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said atoms, as an electrostatic factor of said corresponding one of said atoms;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of said atoms;

deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said atoms, as a steric factor of said corresponding on of said atoms;

assuming that said space occupied rate, said electrostatic factor and said steric factor are

reaction characteristic values of said corresponding one of said atoms,

deriving the reaction characteristic values for all the atoms of a predicting molecule of which a reaction characteristic is to be predicted,

forming a predicting vector having a plurality of vector components selected from the reaction characteristic values of the predicting molecule,

selecting a plurality of data molecules. a reaction characteristic of each of the data molecules being known,

deriving the reaction characteristic values for all the component spaces of each of the data molecules.

forming a data vector for each of the data molecules, the data vector being corresponding to the predicting vector and having a plurality of vector components selected from the reaction characteristic values of each of the data molecules,

estimating a Euclid distance between the predicting vector and each data vector and getting a plurality of Euclid distances between the predicting vector and all the data molecules; and

predicting the reaction characteristic of the predicting molecule to be that the reaction characteristic of the predicting molecule is more similar to a reaction characteristic of a data molecule related to a shorter Euclid distance.

19. (Cancelled)

20. (Previously Presented) A computer-readable storage medium having stored a program for predicting a reaction characteristic of a molecule, said program carrying out a process comprising the steps of:

setting a molecule surrounding surface surrounding the molecule so as to be reflected in a spatial dimension of a molecule, and assuming that a space surrounded by said molecule surrounding surface is a molecule surrounding space;

dividing said molecule surrounding space into a plurality of component spaces, by which a reaction characteristic of said molecule is characterized, in accordance with a predetermined space dividing procedure, and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces, said molecule surrounding space being divided so as that each component space of the plurality of component spaces includes therein each one atom composing

the molecule;

assuming that a portion of each of said component surrounding surfaces appearing outside on said molecule surrounding surface is a frontier surrounding surface of each of said component spaces;

providing probe points on said frontier surrounding surface of each of said component spaces at regular intervals;

deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said electorstatic energies on said frontier surrounding surface of a corresponding one of said component spaces;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said component spaces as a steric factor of said corresponding one of said component spaces; and

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces,

deriving the reaction characteristic values for all the component spaces of a predicting molecule of which a reaction characteristic is to be predicted,

forming a predicting vector having a plurality of vector components selected from the reaction characteristic values of the predicting molecule,

selecting a plurality of data molecules, a reaction characteristic of each of tae data molecules being known,

deriving the reaction characteristic values for all the component spaces of each of the data molecules,

forming a data vector for each of the data molecules, the data vector being corresponding to the predicting vector and having a plurality of vector components selected from the reaction

characteristic values of each of the data molecules,

estimating a Euclid distance between the predicting vector and each data vector and getting a plurality of Euclid distances between the predicting vector and all the data molecules, and

predicting the reaction characteristic of the predicting molecule to be that the reaction characteristic of the predicting molecule is more similar to a reaction characteristic of a data molecule related to a shorter Euclid distance.

21. (New) A molecular reaction characteristic predicting method for predicting n reaction characteristic of a molecule, said method consisting essentially of the steps of:

setting a molecule surrounding surface surrounding the molecule so as to be reflected in a spatial dimension of the molecule, and assuming that a space surrounded by said molecule surrounding surface is a molecule surrounding space;

dividing said molecule surrounding space into a plurality of component spaces, by which a reaction characteristic of said molecule is characterized, in accordance with a predetermined space dividing procedure, and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces, said molecule surrounding space being divided so that each component space of the plurality of component spaces includes therein each one atom composing the molecule;

assuming that a portion of each of said component surrounding surfaces appearing outside on said molecule surrounding surface is a frontier surrounding surface of each of said component spaces;

providing probe points on said frontier surrounding surface of each of said component spaces at regular intervals;

deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said electrostatic energies un said frontier surrounding surface of a corresponding one of said component spaces, as an electrostatic factor of said corresponding one of said component spaces;

deriving van der Waals energies between a probe atom, which is set at each of said probe

points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said component spaces, as a steric factor of said corresponding one of said component spaces;

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces,

deriving the reaction characteristic values for all the component spaces of a predicting molecule of which a reaction characteristic is to be predicted,

forming a predicting vector having a plurality of vector components selected from the reaction characteristic values of the predicting molecule,

selecting a plurality of data molecules; a reaction characteristic of each of the data molecule being known,

deriving the reaction characteristic values for all the component spaces of each of the data molecules,

forming a data vector for each of the data molecules, the data vector being corresponding to the predicting vector and having a plurality of vector components selected from the reaction characteristic values of each of the data molecules,

estimating a Euclid distance between the predicting vector and each data vector and getting a plurality of Euclid distances between the predicting vector and all the data molecules, and

predicting the reaction characteristic of the predicting molecule to be that the reaction characteristic of the predicting molecule is more similar to a reaction characteristic of a data molecule related to a shorter Euclid distance.

Amendments to the Drawings:

The sheets of drawings which are attached after page 18 of this paper form a complete set of Figs. 1 to 4 and include a translation of the Japanese language in Figs. 3 and 4 into English. No new matter has been introduced.

Attachment: Replacement Sheets
Annotated Sheets Showing Changes